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Thermodynamic properties of 2-methyl lactic acid

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ABSTRACT

The measurements of the values of the enthalpy of formation, vaporisation, sublimation and fusion of 2-methyl lactic acid have been performed using methods of combustion calorimetry, transpiration method and differential scanning calorimetry. A conformational analysis has been conducted to identify a set of stable conformers of the compound. Methods of statistical thermodynamics have been used to calculate the thermodynamic functions of the acid in the ideal gas state considering the contribution of the internal rotation in "rigid rotator – *anharmonic* oscillator" approximation within temperature interval (298.15–1500) K for the conformers under study.

1. Introduction

2-Methyl-lactic acid (CAS 594-61-6) is an alpha-hydroxyacid being a methylated derivative of lactic (2-hydroxypropanoic) acid. Similarly, to lactic acid, strong intramolecular interactions between the hydroxyl group located in the alpha position and the carbonyl or hydroxyl oxygen of the carboxyl group can be possibly formed in this compound. Therefore, in our opinion, the considered compound is an important experimental unit in accomplishing one of the main tasks of the physical chemistry – establishing a "structure-property" relationship. A distinct structure of the acid, specifically, the presence of a strong intramolecular interaction supports this ability. Previously, QSPR was incorporated in a study of the thermodynamic properties of a number of oxy- and hydroxyl-carboxylic acids and their esters: lactic acid [1], levulinic acid [2], pyruvic acid [3], methyl-, ethyl- and butyl-esters of levulinic acid [4]. The enthalpies of formation and phase transitions (vaporisation, fusion and sublimation) of these acids have been measured experimentally. A reliable set of the enthalpy properties of examined acids has been formed [1–3]. The thermodynamic parameters of the esterification reactions of levulinic acid have been identified [4].

As continuation of the sequence of studies targeting thermodynamic properties of oxy- and hydroxy-carboxylic acids and their esters, the thermodynamic properties of 2-methyl-lactic acid have been investigated in this work. The combustion calorimetry method has been used to measure the values of the enthalpy of combustion and formation of a crystalline acid. The temperature dependences of the vapour pressure of the substance in the interval 313–380 K have been obtained by the transpiration method. The temperature and the value of enthalpy of fusion have been measured. The value of enthalpy of formation of the acid in a gaseous state has been computed based on obtained results. The reliability of this value has been validated using quantum chemical calculations. The conformational composition of the acid has been tested. According to computed vibrational spectra of the acid, a set of fundamental vibrational frequencies of a substance has been established. The thermodynamic functions of methyl-lactic acid in the ideal gas state in the range (298.15–1500) K have been computed in "rigid rotator – *anharmonic* oscillator" approximation by taking into account mole fractions of the conformers.

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